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MRC Technical Summary Report #2466

QUASIRESONANCE OF LONG LIFE

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January 1983

(Received December 27, 1982)

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QUASIRESONANCE OF LONG LIFE

R. E. Meyer

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ABSTRACT

Schroedinger's equation for a spherically symmetrical potential with central well surrounded by a barrier is studied in the tunneling range of energies, where it possesses states of very long life and correspondingly large, resonant response. The analysis is based on asymptotics with respect to the long life and large response, related to asymptotics of exponential precision, and leads to simple predictions for life and response.

AMS(MOS) Subject Classification: 41A60, 34E20

Key Words: Central scattering, Shortwave asymptotics, Exponential-precision asymptotics

Work Unit Number 2 - Physical Mathematics

Sponsored by the United States Army under Contract No. DAAG29-80-C-0041. The work was supported partially by the National Science Foundation under Grant No. MCS-8001960.

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SIGNIFICANCE AND EXPLANATION

For quantum scattering in a potential with central well surrounded by a barrier, bound states are well-known to be possible at low energies, but not to exist in the tunneling range of energies. Careful spectroscopy, however, has revealed some of the sharpest, apparent resonances just in the tunneling range, and this has attracted interest in quantum chemistry because it suggests a possibility of chemical reactions, even at quite significant rates, the very existence of which quantum mechanics has completely discounted. Those observations have therefore raised a question whether an understanding of such phenomena could open up a new field of non-standard chemistry with major practical implications, if effective ways of generating such novel reactions could be predicted.

The study here reported focuses on the simple case of two-body scattering because it already exhibits the salient features of the phenomenon and the theoretical and practical difficulties characteristic of it. It also focuses directly on those quasis resonances which are likely to have practical significance on account of a large response to radiation excitation. Huge response is indeed found to be possible for quite common types of potentials, but the response is extremely frequency-sensitive, and its observation and exploitation therefore depends on an extraordinary measure of frequency control. This same feature raises great obstacles to theoretical approaches by direct computation and by many familiar analytical methods, but recent results on exponential-precision asymptotics are used in the present investigation to obtain rigorous, and quite simple, predictions of those quasis resonant frequencies, frequency-tolerances and response levels which are associated with high radiation excitation.

Apart from the intriguing vistas for practical chemistry, the phenomenon is also of deeper scientific interest because it necessitates rather radical departures from conventional quantum mechanics. The operators of quasis resonance are not self-adjoint and their study therefore requires new points of view. The present analysis may help, in particular, to illuminate the transition from essentially self-adjoint to frankly non-selfadjoint quantum mechanics.

The responsibility for the wording and views expressed in this descriptive summary lies with MRC, and not with the author of this report.

QUASIRESONANCE OF LONG LIFE

R. E. Meyer

1. Introduction

In central scattering with potential barrier, bound states cannot exist in the tunneling range of energy, but spectroscopy shows that some of the sharpest resonances can, nevertheless, arise in just that range. They are due to inward tunneling, which is a highly effective mechanism for the excitation of quasi-stationary states that, without such radiative input, would decay slowly. Indeed, the decay time or "life" of the wave functions in the absence of excitation, is a measure of the resonant response, whence the main physical interest centers, and the following focuses, on those of very long life.

They arise from eigenstates of complex, but near-real energy, and the height and width of the spectral peak observable are, respectively, roughly inversely and directly proportional to the imaginary part of the eigenvalue, so that wave functions are really needed only in an abstract sense. The search for such eigenvalues of long life, on the other hand, is clearly an asymptotic undertaking with respect to the life as large parameter.

Our approach is therefore different from, and complementary to, the rotation method of Balslev, Combes and Simon¹ and it leads to simple, explicit formulae for the life and response and to an enhanced understanding of the features of the potential which promote long life. The key feature will emerge to be the occurrence of wavelengths of imaginary part small compared with the barrier width at the energy level in question, and this gives a

Sponsored by the United States Army under Contract No. DAAG29-80-C-0041. The work was supported partially by the National Science Foundation under Grant No. MCS-8001960.

natural prominence to quasiclassical notions. They fail at some junctures, however, and to avoid such pitfalls, the analysis is conducted along rigorous lines.

It focuses on two-body scattering both because this illuminates the meaning of quasisresonance most clearly and because it already raises a main difficulty: eigenvalues then exist of imaginary part so painfully small that asymptotics of exponential precision is needed to pinpoint them. Fortunately, it can benefit from results on precision scattering obtained at the hand of an oceanographical problem². They are explained in Section 4, after the scope of the investigation is outlined and the eigenvalue problem, formulated (Sections 2, 3).

Since the eigenstates of interest are quasi-stationary, they are not³ (pp. 33-34, 134) in the customary Hilbert spaces, indeed, the wave functions grow exponentially in the far field (Section 4). The nature of the quantum process is then simplified and illuminated by admission that the operator is non-selfadjoint. The objective of the following, moreover, is not a qualitative description of the whole spectrum, but a quantitative prediction of those eigenvalues which are of practical interest because they have a long life and can be sharply excited. The customary space-and-operator language therefore loses some of its usefulness and a more elementary language³ will serve better. Since precision of quantitative approximation becomes important in quasisresonance, on the other hand, it is difficult to avoid intrusion of some asymptotic terminology^{2,8} in Sections 4-6.

Significant differences in analysis and results arise from the influence of the angular momentum, and the analysis of central reflection is first set out (Section 5) for the case of very large angular momentum, where it is quasiclassical. For relatively small angular momentum (Section 6), the

singularity of the potential (assumed of Coulomb type, for simplicity) dominates the central reflection process and requires recourse to concepts of uniform approximation.

The determination of the eigenvalues of long life in Section 7 is followed by a discussion of the results and some of their limitations (Section 8).

2. Formulation

In central scattering according to Schroedinger's equation,

$$\frac{\hbar^2}{2m} \nabla^2 \Psi + [E - U(r)] \Psi = 0$$

for a wave function $\Psi \exp(-iEt/\hbar)$ in a spherically symmetric potential $U(r)$, it is traditional³ to split off the angular momentum by the help of spherical harmonics $Y_{\ell m}$ so that $\Psi = r^{-1} \psi(r) Y_{\ell m}$ and $\psi(r)$ satisfies a radial Schroedinger equation,

$$\frac{\hbar^2}{2m} \frac{d^2 \psi}{dr^2} + [E - U_{\ell}(r)] \psi = 0, \quad U_{\ell} = U(r) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}.$$

The following concerns potentials of the type indicated in Fig. 1: smooth, with precisely one maximum (say, $U = U_m$ at $r = r_m$), tending as $r \rightarrow \infty$ to a limit $< U_m$ (which will be taken as $U = 0$) and with a central singularity of Coulomb type,⁴

$$rU(r) \rightarrow -U_* < 0 \quad \text{as} \quad r \rightarrow 0. \quad (1)$$

Such barrier potentials possess an inherent, non-dimensional wavenumber scale

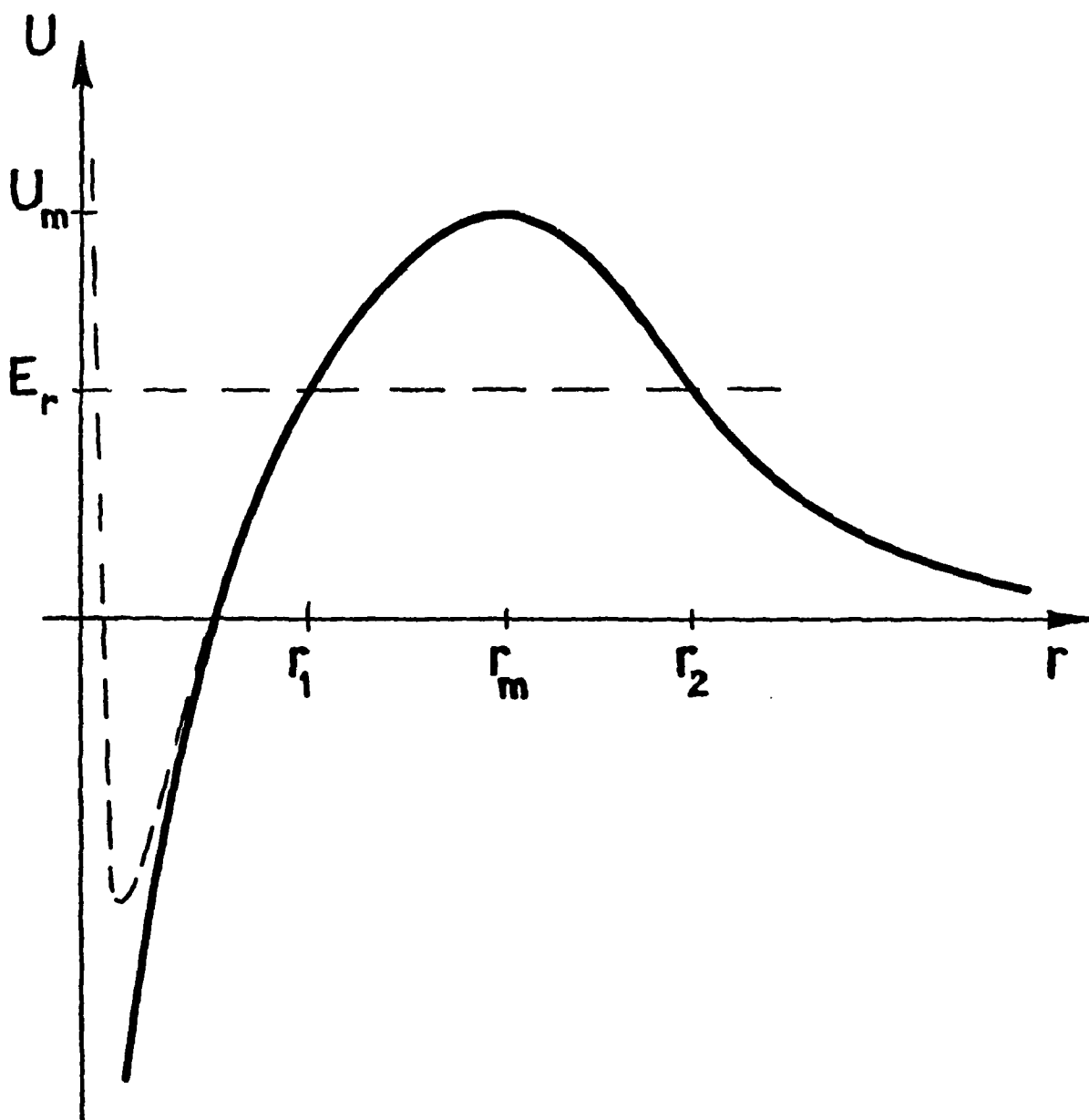
$$k = (2mU_m)^{1/2} r_m / \hbar \quad (2)$$

and if the well radius r_m , barrier height U_m , and \hbar/U_m be chosen as the respective units of length, energy and time, the Schroedinger equation takes the nondimensional form

$$\psi'' + k^2 (E - U_{\ell}) \psi(r) = 0, \quad U_{\ell} = U(r) + \ell(\ell+1)/(kr)^2. \quad (3)$$

Attention will be restricted to angular momenta for which

$2\ell(\ell+1)/k^2 < \max(r^3 dU/dr)$ so that $U_{\ell}(r)$ also possesses a well, and to positive energies below the maximum potential, $0 < E < 1$.



Under such circumstances, the tunneling effect is well known to preclude bound states and to imply time-decay for the wave functions (so that the energy range envisaged is really, not $0 < E < 1$, but $0 < \text{Re } E < 1$). Spectroscopic evidence indicates, however, that such potentials may be associated with states of long "life"

$$T = -\hbar/(\text{Im } E) . \quad (4)$$

which are of primary physical interest because⁵ they possess a sharply "quasiresonant" character. Their study, on which the present investigation focuses, must of necessity involve the asymptotic notion $T \rightarrow \infty$. The question, of course, is how that notion relates to a given potential, and one objective of the following is to show that it is largely interpretable in terms of the notion $k \rightarrow \infty$.

This is plausible, since excitation by tunneling is more effective with wider barriers, and "wide" can have an intrinsic interpretation only in terms of wavelengths. The plausibility stops a little short, however, when it is recalled that there are no waves in a barrier and that the formal scale k is not likely to be representative of the wavenumbers in all important parts of the field. All the same, (2) is a natural, large scale associated with the problem and the cautionary implication is mainly that uniform applicability of the quasiclassical approximation is not thereby assured.

Since the time-decay resulting from tunneling must be associated with complex values of the energy, the roots of $E - U_\ell(r)$ or $E - U(r)$, which are the turning points marking the boundary of the potential barrier, must also be complex. Their central importance⁴ to the character of the Schroedinger equation (3) makes it logical not to ignore them and hence, to give consideration also to complex values of the radius. The key point

emerging from this is that a rational and direct theory of quasisresonance of long life must necessarily involve an analysis in two complex variables, E and r , in addition to asymptotics with respect to a real parameter such as T or k .

To implement this, the potential $U(r)$ needs extension into the complex plane of r , and the simplest expedient is to envisage an analytic potential. Of two grounds on which that appears justified, one is that the observational evidence is unlikely to distinguish between a smooth potential in C^∞ and a sufficiently close, analytic approximation to it. The other is that related work on adiabatic invariance^{6,7} indicates approximation by analytic functions to furnish the most effective approach to a theory of precision-scattering for general potentials in C^∞ . In short, the analytic case is central, and also the most illuminating case.

On the other hand, the complex extension needed is notably economical: $U(r)$ will be assumed analytic on a neighborhood of $(0, \infty)$, however narrow, beyond which it is left undefined. A sectorial character¹ of the domain will not be required.

3. Eigenvalue Problem

The analysis of quasi-stationary states is best related to certain wave functions of clear-cut physical character. Fig. 2 shows the structure of the complex r -plane. For real energy in the tunneling range, $E \sim U_\ell(r)$ in (3) has three real roots r_0 , r_1 , and r_2 , and for decaying states of long life, those roots remain close to the real r -axis, by (4). The figure also shows the "Stokes lines" of (3) on which

$$\operatorname{Re} \int_{r_s}^r [U_\ell(r') - E]^{1/2} dr' = 0, \quad s = 0, 1 \text{ or } 2,$$

and of which three issue from each of the simple roots r_s . Their relevance stems from the theorem⁸ that to each Stokes line L_i corresponds a fundamental solution pair $u_i(r)$, $v_i(r)$ of (3) which have on L_i the character of progressive waves, undamped and un-amplified with distance from r_s . To fix the ideas, u_i will denote the wave outgoing from r_s along L_i and v_i , the wave incident towards r_s . Both are exact solutions of (3) on the whole domain of $U(r)$, but they do not possess the undamped, progressive character on L_j for $j \neq i$.

The fundamental pairs of physical interest are u_0 , v_0 and u_∞ , v_∞ , the respective progressive waves on the central Stokes line L_0 and the far-field Stokes line L_∞ (Fig. 2), because these lines coincide, for real energy, with segments (r_0, r_1) and (r_2, ∞) of the real r -axis, where then

$E - U_\ell(r) > 0$. For long life (4), they depart only little from the real axis and the simple character of the respective fundamental pairs on L_0 and L_∞ remains symptomatic of the main features of their more complicated character on the real-axis segments nearby (Section 4). This indicates the correct formulation of the radiation condition of quasi-stationary states³ (p. 134)

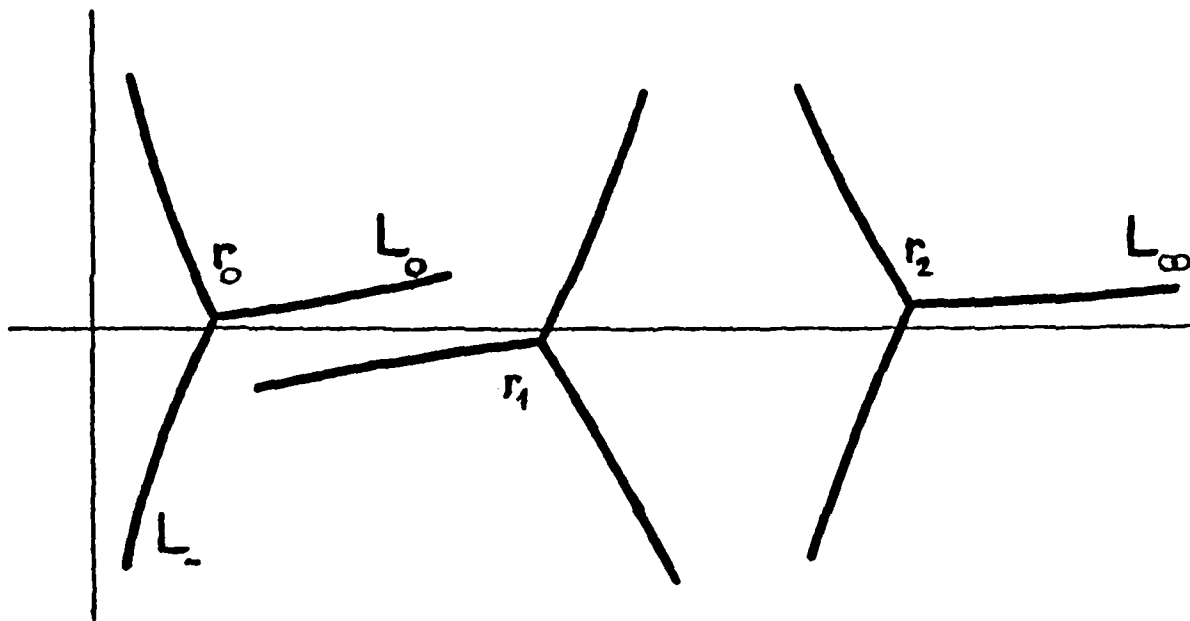


Figure 2. Turning points and Stokes lines in the complex plane of the radius r .

that the wave function represent an outgoing wave in the far field: the representation

$$\psi(r) = A_{\infty} u_{\infty}(r) + B_{\infty} v_{\infty}(r) \quad (5)$$

of the (reduced) wave function as a linear combination of u_{∞} , v_{∞} must satisfy

$$B_{\infty} = 0, \quad A_{\infty} \neq 0. \quad (6)$$

As a result of this radiation condition, the wave functions cannot be relied upon³ (pp. 33-34, 134) to be square-integrable in the far field (Section 4) (and the language of Hilbert space loses some of its customary usefulness). The reflection process in the inner well (Fig. 1), however, is subject to the less global condition³ (p. 103) that the total probability within the well-region be finite, so that $\psi(r) \in L^2(0, r_m)$. The wave-effect of this regularity condition is best described in terms of the central representation,

$$\psi(r) = A_0 u_0(r) + B_0 v_0(r) \quad (7)$$

in which this condition will determine (Sections 5, 6) the ratio

$$A_0/B_0 = R \quad (8)$$

naturally interpretable as the (amplitude) reflection coefficient at the inner barrier set up by the 'centrifugal' effect of the angular momentum in (3).

Since the fundamental pairs are exact solutions of (3) in the whole domain of $U(r)$, they must be linearly related,

$$\begin{bmatrix} u_0(r) \\ v_0(r) \end{bmatrix} = M \begin{bmatrix} u_{\infty}(r) \\ v_{\infty}(r) \end{bmatrix}$$

with constant matrix M . Since (5) and (7) represent the same wave function $\psi(r)$, it follows that the amplitude coefficients are also linearly related,

$$\begin{bmatrix} A_{\infty} \\ B_{\infty} \end{bmatrix} = S \begin{bmatrix} A_0 \\ B_0 \end{bmatrix}$$

with a "scattering matrix" $S(E, k) = ((S_{ij}))$. The exact eigen-condition for quasi-stationary states can therefore be written as

$$\begin{aligned} 0 &= B_{\infty}/B_0 = S_{22} + S_{21}A_0/B_0 \\ &= S_{22} + S_{21}R. \end{aligned} \quad (9)$$

The relevance of this quasi-stationary eigenvalue problem may be illuminated further by the question: what stationary states could occur in the laboratory, which operates at real E and r ? The fundamental pairs u_0 , v_0 and u_{∞} , v_{∞} then describe pure progressive waves, and as a solution of (3), the reduced wave function $\psi^*(r)$ of a stationary state must again be a linear combination,

$$\psi^*(r) = A_0^* u_0(r) + B_0^* v_0(r) = A_{\infty}^* u_{\infty}(r) + B_{\infty}^* v_{\infty}(r).$$

If the wave pairs are normalized appropriately, $|A_i^*|^2$ and $|B_i^*|^2$ represent the outward and inward probability-flux densities³, respectively. To set up such a stationary state, the radiation damping due to outward tunneling must be compensated by incident radiation from 'infinity', so that $B_{\infty}^* \neq 0$.

Comparison of the fluxes $|B_{\infty}^*|^2$ and $|B_0^*|^2$ will then yield a measure

$$|\rho(E, k)|^2 = |B_0^*/B_{\infty}^*|^2$$

of the probability level in the well for unit intensity of incident radiation in the far field. It is a standard measure of the response to excitation (even if only a conservative upper bound, because it presumes long action of a spherically symmetrical, incident radiation).

Since the wave pairs are related by the matrix M , the starred amplitudes must again be related by the scattering matrix $S(E, k)$, and by (9), the amplitude amplification

$$\rho(E, k) = B_0^*/B_{\infty}^* = (S_{22} + S_{21}R)^{-1}.$$

For most real E , $|\rho|$ is quite small (Section 7), but exceptions arise near any near-real roots E_n of (9), where $|\rho| \propto |E - E_n|^{-1}$.

Quasi-stationary eigenvalues E_n of long life therefore predict strong, narrow spectral lines of quasisresonance.

The search for those eigenvalues, on the other hand, is seen from (9) to involve, not the question of approximation of wave functions, but the 'connection'-question how fundamental wave pairs are related to each other. The only way that Schroedinger's equation enters into the quasisresonance problem is through the three coefficients in (9), and the concern of the following must be with adequate approximation of their dependence on E and $U(r)$ when k is large. This is of necessity a somewhat technical matter, and the Reader may wish to skip the next three Sections to find out first what their content is needed for and why adequacy of approximation turns out to make such severe demands.

4. Precision scattering

The computation of the asymptotic expansions of scattering coefficients in powers of k^{-1} is precisely the objective of turning-point connection theory^{8,9} and its application leads to

$$\begin{aligned} \gamma_0 S_{21} &\sim i + \sum_1^{\infty} c_s(E) k^{-s} \\ \gamma_0 S_{22} &\sim \exp[-2k\xi_0(E)] \left\{ 1 + \sum_1^{\infty} d_s(E) k^{-s} \right\} \end{aligned} \quad (10)$$

as $k \rightarrow \infty$, where ξ_0 denotes a familiar WKB wave-distance specified in (13) below and the common factor $\gamma_0 \neq 0$ is irrelevant to the eigencondition (9). However, not only are the c_s and d_s difficult to evaluate for $s > 1$, but it will emerge that such a result fails to yield any information on the life T .

Lozano and Meyer² therefore recalculated S_{21} and S_{22} from the same theory⁹ and showed that, if the question of computing the quantitative content of the symbols be postponed, then these coefficients can be represented by

$$\gamma_0 S_{21} = i \exp\{i \Sigma_1(E, k)/k\} - (1+i) \left\{ 1 + \Omega(E, k)/k \right\} e^{-2k\xi_1} \quad (11)$$

$$\gamma_0 S_{22} = e^{-2k\xi_0} \exp\{i \Sigma_2(E, k)/k\} \quad (12)$$

where Σ_1, Σ_2 represent the functions expanded in (10), Ω denotes a similarly expandable function, and ξ_1 , a less familiar wave distance specified in (14) below. The second term on the righthand side of (11) had not been given before because $\text{Re } \xi_1 > 0$ so that this term is meaningless in the standard, technical sense (10) of asymptotics. The coefficient $E - U_g(r)$ of (3), however, is clearly an analytic function of E and,

according to the principle of conservation of probability³, is real when E and r are real. It follows² that some of the wave solutions u_i, v_i can be defined with a complex-conjugate symmetry in the r - and E -planes, which is inherited by some of their functionals. By reorganizing the long turning-point connection calculations accordingly and tracing these properties of analyticity and complex E -symmetry painstakingly through them, Lozano and Meyer proved² the following.

Precision Scattering Theorem². The scattering coefficients S_{21} and S_{22} in (9) can be represented exactly in the form (11), (12) with

$$\xi_0(E, k) = \int_{r_0}^{r_1} [F_0(r)]^{1/2} dr \quad (13)$$

$$F = U_g(r) - E$$

$$\xi_1(E, k) = - \int_{r_1}^{r_2} [F_1(r)]^{1/2} dr, \quad (14)$$

where the subscripts on F denote a consistent determination of branches of the root, and with $\xi_j(E, k)$ analytic in E and real for real E , and ξ_j and $\Omega(E, k)$ bounded as $k \rightarrow \infty$.

As a corollary, the first term on the righthand side of (11) is seen to be of exactly unit magnitude when E is real, so that the 'very small', second term then describes the whole deviation of $|\gamma_0 S_{21}|$ from unity, regardless of any 'much larger' uncertainties about $\arg(\gamma_0 S_{21})$. One thrust of the theorem is therefore that analyticity in E and the principle of conservation of probability permit us to filter certain exponentially small scattering contributions reliably out of the (algebraic) asymptotic expansions (10). Since these contributions will turn out to determine the life T , the

standard, technical meaning of asymptotically larger and smaller is seen to be somewhat misleading in regard to quasisresonance.

Such considerations reduce the importance of the asymptotic expansions (10) for scattering and instead, direct attention to the WKB-integrals (13), (14). A consistent scheme of branches has been described² in detail for an equation analogous to (3). The main issue is that an analytic continuation of the fundamental wave pairs must be established along a chain of overlapping domains on each of which those functions have a coherent approximation. The procedure of Lozano and Meyer² was to construct such a chain below the turning points r_1, r_2 in the r -plane (Fig. 2), and determinations of (13), (14) consistent with the theorem were thus shown to be $\arg F_0 = \pi$ and

$\arg F_1 = 2\pi$ at real energy, with extension by continuity to slightly complex energy. At real energy, therefore, $k\xi_0 \exp(-i\pi/2) > 0$ and may be interpreted in the familiar way as the width of the potential well of U_ℓ at the level $\text{Re } E$ in units of local, radial wavelengths. Similarly, $k\xi_1 > 0$ at real energy and -- if the potential barrier were not just the place where there are no waves -- should be interpreted as the barrier width of U_ℓ in such units.

The scattering analysis also provides a check on the radiation condition (6). The WKB-approximation to u_∞ is

$$u_\infty(r) \sim c_\infty F_\infty^{-1} \exp[k\xi_\infty(r)], \quad \xi_\infty(r) = \int_{r_2}^r [F_\infty(s)]^{1/2} ds$$

where c_∞ denotes a normalization factor and $F_\infty(r)$, the branch of the function F in (13), (14) appropriate to the far field. The determination consistent with those just mentioned is² $\arg F_\infty = \pi$ on L_∞ , and as $r \rightarrow \infty$ along the real axis, where $U_\ell(r) \rightarrow 0$, this gives $\xi_\infty \sim E^{1/2} r \exp(i\pi/2)$. The phase of the full, far-field wave function $A_\infty r^{-1} u_\infty Y_{\ell m} \exp(-iEt)$ is therefore

$$\text{Im}\{k\xi_{\infty} - iEt\} \sim kr \text{Re } E^{1/2} - t \text{Re } E$$

as $r \rightarrow \infty$ along the real axis, and this describes an outgoing wave for $\text{Re } E > 0$, as it must be in the tunneling range. The radiation condition (6) therefore implies the intended wave character in the far field even if L_{∞} should leave the domain. However,

$$\text{Re}\{k\xi_{\infty} - iEt\} \sim t \text{Im } E - kr \text{Im } E^{1/2}$$

as $r \rightarrow \infty$ along the real axis and for positive life (as it will be seen in Section 7 to be predicted by (9)) the wave function decays both at fixed position and at fixed phase, but at fixed time, it grows with increasing r . While this mathematical growth is exponential and precludes convergence of $\int |\psi|^2 dr$, the magnitude of $k \text{Im } E^{1/2}$ will emerge in Section 7 to be so small, that the growth may be hard to observe at realistic distances.

5. Reflection: large angular momentum

In the computation of the reflection coefficient (8), a distinction between large and small angular momentum appears unavoidable and it is convenient to begin with the case of quantum numbers ℓ so large that

$$\mu^2 = \ell(\ell+1)/k^2$$

can be regarded as independent of k . Then U_ℓ in (3) is independent of k and only a more precise version of quasiclassical analysis^{4,10} is required. When $2\mu^2 < \max_{r \in \mathbb{R}} (r^3 dU/dr)$, $U_\ell(r)$ still possesses a well and quasisresonance may occur at energies of real part between $\min U_\ell$ and $\max U_\ell$, to which attention will therefore be restricted. All three roots r_0, r_1, r_2 of $F(r) = U_\ell(r) - E$ are now independent of k . The branches chosen for (13), (14) are based on $\arg F'_0(r_0) = \pi$ for real E and are consistently extended by $\arg(r - r_0) = -\pi$ for real $r \in (0, r_0)$ (Fig. 2) to match the analytic continuation of Section 4 passing below the turning points in the r -plane. The domains of validity of simple asymptotic approximations to solutions of (3) are restricted by conditions¹¹ that prevent the domain D_0 containing the Stokes line L_0 (Fig. 2) from reaching points in $(0, r_0)$, where the regularity condition can be plainly interpreted. To reach them, the domain D_- of L_- (Fig. 2) is needed, which lies below r_0 and overlaps with D_0 . The branch F_- of F appropriate for L_- has $\arg F'_-(r_0) = 3\pi$ for real energy and the corresponding wave variables

$$\begin{aligned} \xi_-(r) &= \int_{r_0}^r [F_-(t)]^{1/2} dt & \text{on } D_- \\ \xi_0(r) &= \int_{r_0}^r [F_0(t)]^{1/2} dt & \text{on } D_0 \end{aligned} \tag{15}$$

are therefore related by

$$\xi_-(r) = \xi_0(r) e^{i\pi} \text{ on } D_- \cap D_0, \quad (16)$$

even at non-real energy. (The function $\xi_0(E, k)$ of Sections 4, 7 is thus seen to be $\xi_0(r_1(E, k))$ in the notation of Sections 5, 6.)

Langer's transformation⁸ of (3) near r_0 is

$$\xi_- = \frac{2}{3} \zeta^{3/2}, \quad \psi(r) = (d\zeta/dr)^{-1/2} w(\zeta)$$

and casts (3) into the form

$$d^2 w/d\zeta^2 = (k^2 \zeta + \phi_-) w$$

with a function ϕ_- satisfying the hypotheses of Olver's⁸ Theorem 9.1 (p. 417). Accordingly, (3) has a fundamental solution pair ψ_r, ψ_s with first approximations

$$\begin{aligned} \psi_r(r) &\sim (d\zeta/dr)^{-1/2} \text{Ai}(k^{2/3} \zeta) \\ \psi_s(r) &\sim (d\zeta/dr)^{-1/2} \text{Bi}(k^{2/3} \zeta) \end{aligned} \quad (17)$$

in terms of standard Airy functions Ai, Bi as $k \rightarrow \infty$, uniformly for bounded $|\zeta|$. In $(0, r_0)$, $\arg \xi_-$ is near zero for near-real energy and the same holds for $\arg \zeta$. Therefore, $\psi_s(r)$ does not yield a wave function square-integrable in the well and only multiples of $\psi_r(r)$ are admissible.

To translate this into information on the central reflection coefficient R requires the representation of $\psi_r(r)$ in terms of the wave pair

$$\begin{aligned} u_0(r) &\sim c_0 F_0^{-1/4} e^{k\xi_0(r)} [1 + O(k^{-1})] \\ v_0(r) &\sim c_0 F_0^{-1/4} e^{-k\xi_0(r)} [1 + O(k^{-1})] \end{aligned} \quad (18)$$

of L_0 (Fig. 2). Since $\arg \zeta = \pi$ on L_0 , that representation can be obtained from the identity⁸

$$-\text{Ai}(k^{2/3} \zeta) = e^{-2\pi i/3} \text{Ai}(k^{2/3} \zeta e^{-2\pi i/3}) + e^{-4\pi i/3} \text{Ai}(k^{2/3} \zeta e^{-4\pi i/3})$$

where the Airy functions on the righthand side then come to be taken at points of argument $\pm \pi/3$ and their standard asymptotic approximation⁸

$$\text{Ai}(z) \sim \frac{1}{2} (\pi^2 z)^{-1/4} \exp\left\{-\frac{2}{3} z^{3/2}\right\} [1 + o(z^{-3/2})]$$

can be used. This yields

$$\begin{aligned} -\text{Ai}[k^{2/3} \zeta] &\sim \frac{1}{2} \pi^{-1/2} k^{-1/6} \zeta^{-1/4} e^{-\pi i/2} \{e^{k \xi_-} [1 + o(k^{-1})] \\ &\quad + e^{-\pi i/2} e^{-k \xi_-} [1 + o(k^{-1})]\} \end{aligned}$$

and accordingly,

$$\begin{aligned} \psi_r(r) &\sim \frac{1}{2} \pi^{-1/2} k^{-1/6} F_-^{-1/4} \{e^{k \xi_0(r)} [1 + o(k^{-1})] \\ &\quad + e^{\pi i/2} e^{-k \xi_0(r)} [1 + o(k^{-1})]\} \end{aligned} \quad (19)$$

on L_0 . Comparison with (7) and (18) now shows

$$R = A_0/B_0 = e^{-i\pi/2} + o(k^{-1})$$

in (8).

This is the result of standard, quasiclassical^{4,10} theory and is again inadequate for information on the life T because its degree of accuracy destroys the chance of using the new information of the Precision Scattering Theorem in the eigencondition (9). Nor would the asymptotic expansion of R help in that respect. By their appeal to conservation of probability, however, Lozano and Meyer² showed that u_0, v_0 can be normalized so that the error terms in (18) are complex-conjugates of each other for real E . As a wave function of (3), $\psi_r(r)$ is similarly normalizable to be real for real E and r , and the error terms in (19) are therefore also complex-conjugates when E is real. It now follows from the comparison of (7), (18) and (19) that $|R| = 1$ exactly for real E and furthermore, since the solutions of (3) depend analytically on E , that

$$R = e^{-i\pi/2} \exp[ik^{-1} \Sigma_0(E, k)] \quad (20)$$

with Σ_0 again analytic in E , bounded as $k \rightarrow \infty$, and real for real E .

6. Reflection: smaller angular momentum

As the angular momentum decreases, the turning point r_0 moves closer to the singular point $r = 0$ of the potential and quasi-classical analysis begins to fail because more careful account must be taken⁴ of this central singularity.

For small $|r_0|$, the Langer transformation for (3) is⁸ to variables

$$\zeta^{1/2} = \int_0^r [f_0(t)]^{1/2} dt, \quad w(\zeta) = (d\zeta/dr)^{1/2} \psi(r),$$

where $f_0(r)$ is a branch of $U(r) - E$. The Schroedinger equation (3) then takes the form⁸

$$d^2 w/d\zeta^2 = \left[\frac{k^2}{4\zeta} + \frac{\ell(\ell+1)}{\zeta^2} + \frac{\phi_0}{\zeta} \right] w$$

where

$$\phi_0/\zeta = \ell(\ell+1) \left[r^{-2} \left(\frac{dr}{d\zeta} \right)^2 - \zeta^{-2} \right] + \left(\frac{dr}{d\zeta} \right)^{1/2} \frac{d^2}{d\zeta^2} \left(\frac{d\zeta}{dr} \right)^{1/2}$$

satisfies the hypothesis of Olver's⁸ Theorem 9.1 (p. 458). Accordingly, (3) possesses a pair of exact solutions ψ_r, ψ_s with approximations in terms of modified Bessel functions I, K ,

$$\begin{aligned} \psi_r &\sim [\zeta/(4f_0)]^{1/4} \{ I_{2\ell+1}(k\zeta^{1/2}) [1 + o(k^{-2})] \\ &\quad + (B_0 \zeta^{1/2}/k) I_{2\ell+2}(k\zeta^{1/2}) [1 + o(k^{-2})] \} \\ \psi_s &\sim [\zeta/(4f_0)]^{1/4} \{ K_{2\ell+1}(k\zeta^{1/2}) + o(|\zeta^{1/2}/k|) \} \end{aligned} \quad (21)$$

as $k \rightarrow \infty$ for fixed ℓ , uniformly in a domain including the Stokes line L_0 (Fig. 2), if

$$\begin{aligned} f_0(r) &= e^{i\pi} |U(r) - E| \\ &\sim e^{i\pi} U_* r^{-1} [1 + (E - U_0)r/U_* + o(r^2)] \quad \text{as } r \rightarrow 0, \end{aligned} \quad (22)$$

by (1). From the properties of the Bessel functions⁸,

$$k^{-2l-1} r^{-l-1} \psi_r \quad \text{and} \quad k^{2l+1} r^l \psi_s$$

are seen to approach nonzero limits as $r \rightarrow 0$ for large k and fixed l .

For angular momentum $l > 1$, ψ_s thus fails to be square-integrable in the well and cannot contribute to the wave functions. For $l = 0$, the definition of reflection will here be complemented by the condition³ (p. 103)

$\psi(0) = 0$, and ψ_r is then also the only admissible solution of (3).

To obtain the exponential precision needed for information on the life T , it will again suffice to combine the exact results quoted with a first approximation to ψ_r on a suitable segment of the Stokes line L_0 (Fig. 2) and to this end, a more precise version of Kramers' analysis⁴ will be adequate. For a simple and direct approach to reflection, attention may be focused on a segment of L_0 on which

$$|r_0| \ll |r| \ll U_*/|E - U_0|.$$

For fixed angular momentum l , the root r_0 of $U_l - E$ is

$$r_0 = \frac{l(l+1)}{k^2 U_*} \left[1 + \frac{U_0 - E}{U_*} \frac{l(l+1)}{k^2 U_*} + O(k^{-4}) \right]$$

by (3) and (22). In terms of $\xi_0(r)$ and of

$$\eta = \xi^{1/2} \exp(-\pi i/2),$$

the segment of L_0 under consideration is therefore seen from (3), (15) and (22) to be one on which

$$|\xi_0| \rightarrow 0 \quad \text{but} \quad k|\xi_0| \rightarrow \infty,$$

$$|\eta| \rightarrow 0 \quad \text{but} \quad k|\eta| \rightarrow \infty,$$

and to cut the story short, it will be chosen so that $k|\xi_0|^2$ is bounded as

$k|\xi_0| \rightarrow \infty$. From (21),

$$\psi_r \sim (\pi k)^{-1/2} f_0^{-1/4} e^{(l+3/4)\pi i} \cos[k\eta - (l + 3/4)\pi + o(|k\eta|^{-1})] \quad (23)$$

on such a segment of L_0 . From (22), in turn,

$$\eta \sim 2(u_{*r})^{1/2} [1 + o(|\eta|^2)]$$

and from (15),

$$\begin{aligned} \xi_0 &= \{2r F_0^{1/2} [1 + o(|k^2 r^2 F_0|^{-1})] - \frac{\pi}{k} e^{i\pi/2} [l(l+1)]^{1/2} \} [1 + o(|r|)] \\ &= e^{i\pi/2} \{ \eta - \frac{\pi}{k} [l(l+1)]^{1/2} + o(k^{-2} |\eta|^{-1}) \} [1 + o(|\eta|^2)] \end{aligned} \quad (24)$$

on such a segment, while $f_0^{-1/4} = F_0^{-1/4} [1 + o(|k\xi_0|^{-2})]$. Therefore, the

ξ_0 -wave representation of ψ_r is there

$$\psi_r \sim (\pi k)^{-1/2} F_0^{-1/4} e^{(l+3/4)\pi i} \cos[k\xi_0 e^{-\pi i/2} - \frac{\pi}{4} - \pi\sigma(l) + o(|k\xi_0|^{-1})] \quad (25)$$

with

$$\sigma(l) = l - \frac{1}{2} - [l(l+1)]^{1/2} \quad (26)$$

and comparison with (8) and (18) shows

$$R = e^{-i\pi(1/2 + 2\sigma)} + o(|k\xi_0|^{-1})$$

This result is again insufficient for any information on the life T , but since the wave function ψ_r is again normalizable to be real for real E and R , it follows again that $|R| = 1$ exactly for real E and therefore

$$R = e^{-i\pi(1/2 + 2\sigma)} \exp[ik^{-1/2} \Sigma_0(E, k)] \quad (27)$$

with still Σ_0 analytic in E , bounded as $k \rightarrow \infty$ and real for real E .

When (27) is compared with (20), the angular-momentum correction to reflection is seen to be⁴ massive for $l = 0$, but to decrease rapidly with increasing l . In the limit discussed in Section 5, (27) approaches (20), and it appears a fair conjecture that (27) holds for all angular momenta. Proof would require filling a gap in the theory of Bessel functions⁸, but the

plausibility of the conjecture is enhanced by noting that the root r_0 of $U_l - E$ moves with increasing l close to the point where order and argument of the Bessel function in (21) are equal, and for large order $2l + 1$, that is a turning point where the Bessel function has an Airy-representation⁸ corresponding to that encountered in (17). A unified representation of the wave function ψ_r for all angular momenta might therefore exist, and it will be seen in the next Section that it would yield a further clarification of the quantization rules. In any case, since (26) gives $2\sigma = 0.056$ already for $l = 4$, the difference, if any, between (26) and the exact angular-momentum correction to the phase shift of reflection can be rarely significant.

Since a uniform approximation of ψ_r up to the central singularity $r = 0$ of the potential (which is not mapped on any ξ_0) is obtainable only in terms of $\zeta^{1/2} = i\eta$, this is the variable used in the mathematical theory⁸. Besides, ξ_0 differs from η only by correction terms tending to zero in the wave region as $k \rightarrow \infty$, and mathematical usage favors simple variables uncontaminated by correction terms. That can be shortsighted, for in terms of η , the wave representation of ψ_r is given already by (23), but the corresponding reflection coefficient,

$$R_\eta = e^{-3\pi i/2} \exp[ik^{-1/2} \Sigma_\eta(E, k)] ,$$

is quite different from (20) and agrees with (27) only for $l = 0$. Its correct use in the eigencondition requires proper account, after all, of the difference between ξ_0 and η in (18).

7. Eigenvalues

When (11), (12) and (27) are substituted in the characteristic form

$$\Delta(E, k) = S_{22} + S_{21}R$$

of (9), it may be split rather naturally into

$$\begin{aligned}\Delta(E, k) &= i\gamma_0^{-1} R\{\Delta_0(E, k) + \Delta_1(E, k)\}, \\ \Delta_0 &= \exp[-2k\xi_0 + 2\pi i\sigma + i\xi_2/k - i\xi_0/k^{1/2}] + \exp(i\xi_1/k) \\ \Delta_1 &= (i - 1)(1 + \Omega/k) \exp(-2k\xi_1)\end{aligned}\quad (28)$$

so that Δ_0 collects all the functions whence asymptotic contributions to Δ of algebraic type in k^{-1} can be anticipated, while Δ_1 can make only an exponentially small contribution when $\text{Re } \xi_1 > 0$. [In (28), ξ_0 denotes again the quantity (13), which is $\xi_0(r_1)$ in the notation of (15).]

To compute the near-real roots of Δ , it is convenient to begin with the real roots E_r of $\Delta_0(E, k)$. Since $\xi_0(E, k) = i|\xi_0|$ for real E , they are given by

$$k|\xi_0(E_r, k)| + (\xi_1 - \xi_2 + k^{1/2}\xi_0)/(2k) = (n + \frac{1}{2} + \sigma)\pi \quad (29)$$

with large integer $n > 0$ below a cut-off n_c . In dimensional notation, this is

$$(2mU_m)^{1/2} \int_{r_0}^{r_1} |E_r - U_\ell(r)|^{1/2} dr = (n + \frac{1}{2} + \sigma) \pi \hbar [1 + O(k^{-3/2})], \quad (30)$$

$$U_\ell(r_0) = U_\ell(r_1) = E_r,$$

where $U_m = \max_{r \in R} U(r)$, U_ℓ is given by (2) and (3), and (r_0, r_1) is the U_ℓ -well interval of the radius at the level E_r . Apart from the angular-momentum correction⁴ σ , (30) is just the quasiclassical description of energy levels ignoring the radiation damping. The new feature that it is an exact version of the quantization rule is not of much direct use because an algorithm for the evaluation of the ξ_1 is available^{8,9} only for an

unrealistically restricted class of potentials. The feature of immediate relevance is that, since $U(r)$ is monotone increasing on $(0, r_m)$ (Fig. 1), (30) is known to determine a unique, real $E_r(n)$ for large k and given integer n such that still $E_r(n) < U_m$.

The quantization correction σ is given by (26) for small angular momentum l and to a good approximation, at least, also for larger l . For $l = 0$, (30) therefore becomes an integer quantization rule, but as $l \rightarrow \infty$, $\sigma \rightarrow 0$, and even for $l = 1$, $\sigma = 0.086$ only. It may be remarked incidentally that the results of Section 6 show that (30) may be rephrased for small angular momentum in terms of the uncorrected potential $U_m U(r)$, and it then becomes an integer quantization rule,

$$(2mU_m)^{1/2} \int_0^{r_1} |E_r - U(r)|^{1/2} dr = (n + 1)\pi \hbar [1 + O(k^{-3/2})] ,$$

$$U(r_1) = E_r - l(l + 1)/(kr_1)^2 .$$

To determine now the eigenvalues in the presence of radiation damping, let a prime denote $\partial/\partial E$ for functions of E and k and note from (13), since $F(r_0) = F(r_1) = 0$,

$$\xi'_0(E, k) = \frac{1}{2} \int_{r_0}^{r_1} [F_0(r)]^{-1/2} (\partial F_0 / \partial E) dr$$

and in particular,

$$\xi'_0(E_r, k) = \frac{1}{2} e^{i\pi/2} \int_{r_0}^{r_1} |E_r - U_l(r)|^{-1/2} dr \neq 0 . \quad (31)$$

Similarly, $\xi'_1(E_r, k)$ exists, so that $\Delta_0(E, k)$ and $\Delta_1(E, k)$ are analytic in E on a neighborhood of $E = E_r(n)$ and $\Delta'_0(E_r, k) \neq 0$, by (29). For

fixed k , accordingly, (29) defines a one-one map between near-disc neighborhoods about the points $E = E_r(n)$ and $k^{-1}\Delta_0 = 0$ in the respective planes of E and $k^{-1}\Delta_0$, and since the k -dependence of $\xi_0(E, k)$ decreases with increasing k , by (13) and (3), those discs approach k -independent sizes as $k \rightarrow \infty$. For sufficiently large k , therefore, the image of the map in the plane of Δ_0 covers any desired neighborhood of $\Delta_0 = 0$. In particular, if N_1 denotes that neighborhood of $E = E_r(n)$ on which

$|\Delta_0| < 2 \exp[-2k\xi_1(E_r, k)]$ only, then N_1 is certain to be in the domain of the map, to have a simple closed curve ∂N_1 as boundary and to contain no root of Δ_0 other than $E = E_r(n)$. Since $|\Delta_1| < |\Delta_0|$ on ∂N_1 , it follows from the principle of the argument that N_1 contains precisely one root of $\Delta_0(E, k) + \Delta_1(E, k)$ and that this root, E_n , is simple.

A simple eigenvalue E_n close to $E_r(n)$ is thereby established for each large enough integer $n < n_c$, and to the first approximation as $k \rightarrow \infty$,

$$E_n - E_r(n) \sim -\Delta_1(E_r, k)/\Delta_0'(E_r, k) \\ \sim -\frac{1}{2} (1 + i) [k |\xi_0'(E_r, k)|]^{-1} \exp[-2k\xi_1(E_r, k)] .$$

The real part of this result has little practical meaning on account of the difficulty of computing $E_r(n)$ from (29) with comparable accuracy. The imaginary part, on the other hand, gives the rigorous, first approximation to $\text{Im } E_n$ as $k \rightarrow \infty$ and the corresponding eigenfunction life

$$T_n = \frac{-\hbar}{U_m \text{Im } E_n} \sim \frac{2\hbar k}{U_m} |\xi_0'(E_r(n), k)| \exp[2k\xi_1(E_r(n), k)] \\ \sim 2(2m/U_m)^{1/2} |\xi_0'(E_r(n), k)| \exp[(8mU_m)^{1/2} \xi_1(E_r(n), k)/\hbar] \quad (32)$$

with $E_r(n)$, ξ_0' and ξ_1 given by (30), (31) and (14).

The salient features of this result are that the life is exponentially large in \hbar and that its computation involves no more than the evaluation of the two definite, WKB-integrals (31), (14), once the real part $E_r(n)$ of

E_n has been determined from the standard quantization rule (30). The latter task, however, requires high accuracy for experimental comparisons because the quasisresonance arises from the exponential closeness of the eigenvalue to the real axis of the energy-plane and hence, the energy-band width of the quasisresonance is an exponentially narrow one centered near $E_r(n)$.

To obtain the response $\rho(E,k) = \Delta(E,k)^{-1}$ to excitation (Section 3) in scattering at real energy requires consideration also of the factor γ_0 in (11), (12), which is $\exp[-k\xi_1(E,k)]\{1 + O(k^{-1})\}$. Thus $|\rho|$ has an exponentially large maximum

$$|\rho|_{\max} \sim \exp[k\xi_1(E_r(n),k)]$$

at each quasisresonant energy-level, but over nearly the whole interval between successive such levels, the response is only of the exponentially small order of its minimum,

$$|\rho|_{\min} \sim \gamma_0 / \max|\Delta_0(E_r, k)| \sim \frac{1}{2} \exp[-k\xi_1(E_r, k)] .$$

The energy-dependence of cross-sections therefore looks as if there were a continuous spectrum with response of order $|\rho|_{\min}$ at most energies in the tunneling range, but with very sharp, 'quasisresonant' peaks of order $|\rho|_{\max}$ near $E_r(n)$.

8. Discussion

The main result of the analysis is rigorous confirmation of the plausible conjecture that the essence of quasisonance of long life is the existence of energy eigenvalues of small imaginary part because of tunneling. The quantization rule (30) and life-formula (32), moreover, give a simple, quantitative prediction of such eigenvalues. They show the main requirement for their occurrence to be the existence of energy levels at which the potential barrier is wide compared with the 'local wavelength'.

A rough estimate of that wavelength is normally given by

$$k^{-1} = \hbar / [2mU_m r_m^2]^{1/2},$$

where \hbar is the usual Planck constant, m is the reduced mass for the elastic, two-particle scattering here studied, U_m is the height of the potential-barrier top above the far-field potential level, and r_m is the total radius of the potential well (Fig. 1). Barriers wide compared with k^{-1} are therefore not uncommon, and a rough idea of the potential suffices for predicting their presence.

When quasisonance is important, moreover, it has been shown to have distinctive features. The life and with it, also the response to radiation excitation at the resonant energy level, is exponentially large in the wave number scale k . The bandwidth of quasisonant excitation, however, is exponentially narrow because the long life arises from the proximity of an eigenvalue to the real energy-axis. This intrinsic coupling of extremely large response with extremely narrow bandwidth characteristic of important quasisonance has considerable practical implications. It would also create difficulties for direct numerical attacks on the Schroedinger equation and enhances the value of the simple predictions obtained here by long-life asymptotics.

A feature of the analysis which may be worth more explicit remark is that it treats a distinctly non-selfadjoint problem of the Schroedinger equation, since it concerns nonreal energy eigenvalues. This feature moves the eigenfunctions out of the customary Hilbert spaces.¹ None the less, the normal quantization rule of the self-adjoint case has been proven to remain applicable because interest for quasisresonance centers on near-real eigenvalues. It may be a good example of the fact that loss of self-adjointness need not generate a discontinuous, quantitative change.

Some further comments on the scope and limitations of the present analysis may also be appropriate. For small or moderate angular momentum, the low-level bound states occur quite deep in the well because (30) shows large quantum numbers n to correspond already to the lowest energy levels of the tunneling range of energies. The present analysis then covers all eigenvalues of long life because it begins to fail only at energy levels so close to the potential-barrier top that the barrier width becomes small. This failure of the analysis therefore only keeps step with shrinkage of the life to relative unimportance.

For very large angular momentum, a failure of the present analysis can occur at the lowest, quasisresonant energy levels. The well of the potential U_l corrected for the 'centrifugal effect' is then relatively shallow and even its bottom may lie in the tunneling range. Low-level quantum states might then occur at levels where the barrier is wide, which would indicate long life, but where the well is narrow. Shortwave analysis would accordingly fail for the well, but would remain applicable to most of the barrier. It then becomes relevant that the present analysis furnishes striking confirmation that typical bound-state analysis can give close approximations to the real parts of eigenvalues even in the tunneling range. This makes it

appear likely that normal methods for the determination of low, bound levels could be combined with shortwave analysis of the barrier, in such cases. If approximations to $\Delta_0(E_r, k)$ and $\Delta'_0(E_r, k)$ be thus obtained from low-level, bound-state analysis or computation, then the results for $\Delta_1(E_r, k)$ of Section 7 would be likely to give approximations to the life whenever quasisresonance is important.

For angular momentum that is large, but not large enough to have a quantum number l comparable to the wavenumber scale k , a modified, quasiclassical analysis is needed, which has not been given, but has been shown to be unlikely to modify the results materially.

Acknowledgments

The author is indebted to Professor P. R. Certain for prompting this work and to both him and Dr. C. Lozano, for good advice.

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4. TITLE (and Subtitle) QUASIRESONANCE OF LONG LIFE		5. TYPE OF REPORT & PERIOD COVERED Summary Report - no specific reporting period
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) R. E. Meyer		8. CONTRACT OR GRANT NUMBER(s) DAAG29-80-C-0041 & MCS-8001960
9. PERFORMING ORGANIZATION NAME AND ADDRESS Mathematics Research Center, University of Wisconsin 610 Walnut Street Madison, Wisconsin 53706		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS Work Unit Number 2 - Physical Mathematics
11. CONTROLLING OFFICE NAME AND ADDRESS See #18 below		12. REPORT DATE January 1983
		13. NUMBER OF PAGES 31
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		15. SECURITY CLASS. (of this report) UNCLASSIFIED
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE
16. DISTRIBUTION STATEMENT (of this Report) Approved for public release; distribution unlimited.		
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)		
18. SUPPLEMENTARY NOTES Sponsored by: U. S. Army Research Office National Science Foundation P. O. Box 12211 Washington, D. C. 20550 Research Triangle Park North Carolina 27709		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number) Central scattering, Shortwave asymptotics, Exponential-precision asymptotics		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) Schroedinger's equation for a spherically symmetrical potential with central well surrounded by a barrier is studied in the tunneling range of energies, where it possesses states of very long life and correspondingly large, resonant response. The analysis is based on asymptotics with respect to the long life and large response, related to asymptotics of exponential precision, and leads to simple predictions for life and response.		

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